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Title (English)

Single-molecule X-ray free-electron laser imaging – Interconnecting sample orientation with explosion data

Title (Swedish)

Abstract

Single-molecule serial femtosecond imaging is a relatively new, emerging discipline of X-ray crystallography eliminating the need of a sample crystal. In this work we used molecular dynamics simulations to determine if the explosion pattern of a molecule undergoing such analysis can provide information regarding its initial spatial orientation.

(Full abstract on page vii)

Keywords

X-ray, free-electron laser, XFEL, diffraction analysis, structure determination, nanocrystal, molecular dynamics, GROMACS, biomolecular imaging, ubiquitin, trajectory, explosion

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